LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082321\
Data File : BF125170.D
Acq On : 23 Aug 2021 23:27
Operator : JU/CG
Sample : M3449-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125170.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	16	23	31	rVB	1153828	1534490	41.22%	5.463%
2	5.151	516	521	526	rVB	109675	139547	3.75%	0.497%
3	5.540	582	587	590	rBV	3627366	3428172	92.08%	12.204%
4	6.545	752	758	761	rBV	3264451	3440548	92.41%	12.248%
5	6.922	818	822	825	rBV	1195321	907534	24.38%	3.231%
6	7.481	912	917	920	rBV	2423090	2231929	59.95%	7.945%
7	8.098	1019	1022	1032	rBV	542064	477278	12.82%	1.699%
8	8.204	1036	1040	1043	rBV	1449468	1162349	31.22%	4.138%
9	9.280	1218	1223	1226	rBV	4410028	3722992	100.00%	13.253%
10	9.957	1335	1338	1342	rBV	1337322	1230133	33.04%	4.379%
11	10.745	1468	1472	1476	rBV	2289979	2185862	58.71%	7.781%
12	11.445	1588	1591	1594	rBV	1278499	1093609	29.37%	3.893%
13	11.469	1594	1595	1598	rVB	88413	56380	1.51%	0.201%
14	11.963	1674	1679	1685	rBV2	383666	402201	10.80%	1.432%
15	12.657	1794	1797	1802	rBV	230995	216947	5.83%	0.772%
16	12.751	1810	1813	1817	rBV	291660	268562	7.21%	0.956%
17	12.892	1832	1837	1841	rBV	179795	196938	5.29%	0.701%
18	13.033	1857	1861	1864	rBV	3547976	3025574	81.27%	10.771%
19	13.927	2010	2013	2020	rBV	190684	313896	8.43%	1.117%
20	14.092	2037	2041	2043	rBV	910104	905586	24.32%	3.224%
21	14.115	2043	2045	2047	rVB	99762	67098	1.80%	0.239%
22	15.145	2216	2220	2223	rBV	151717	258858	6.95%	0.921%
23	15.592	2291	2296	2299	rBV	625467	824747	22.15%	2.936%

Sum of corrected areas: 28091230

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Misc :
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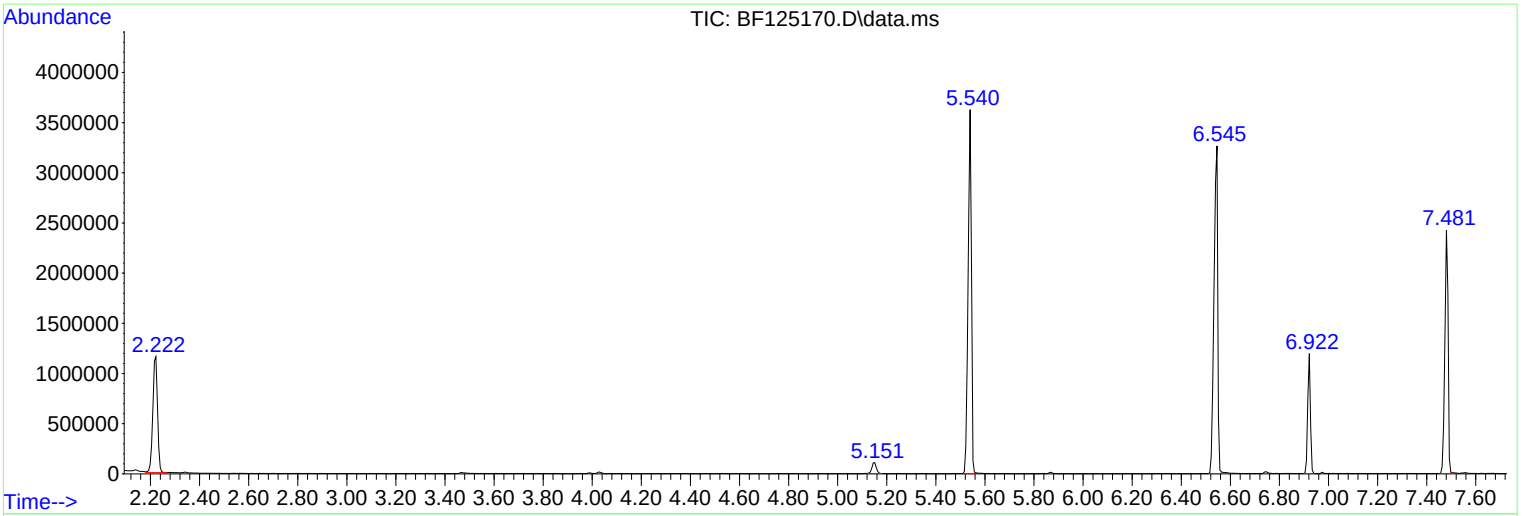
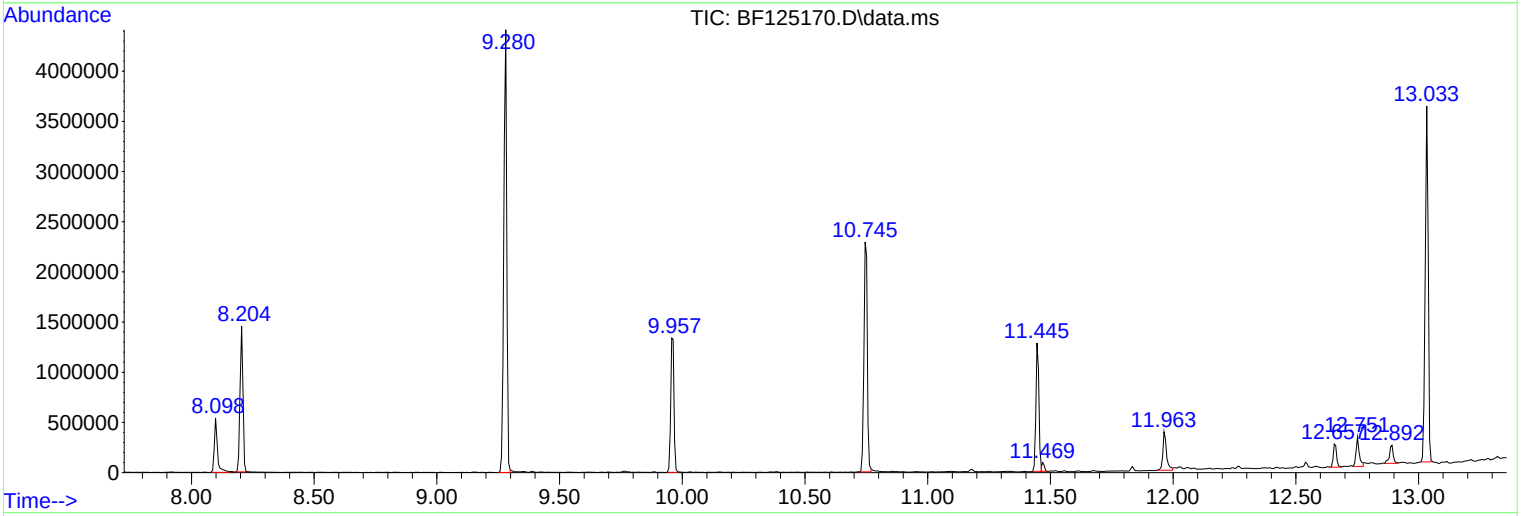
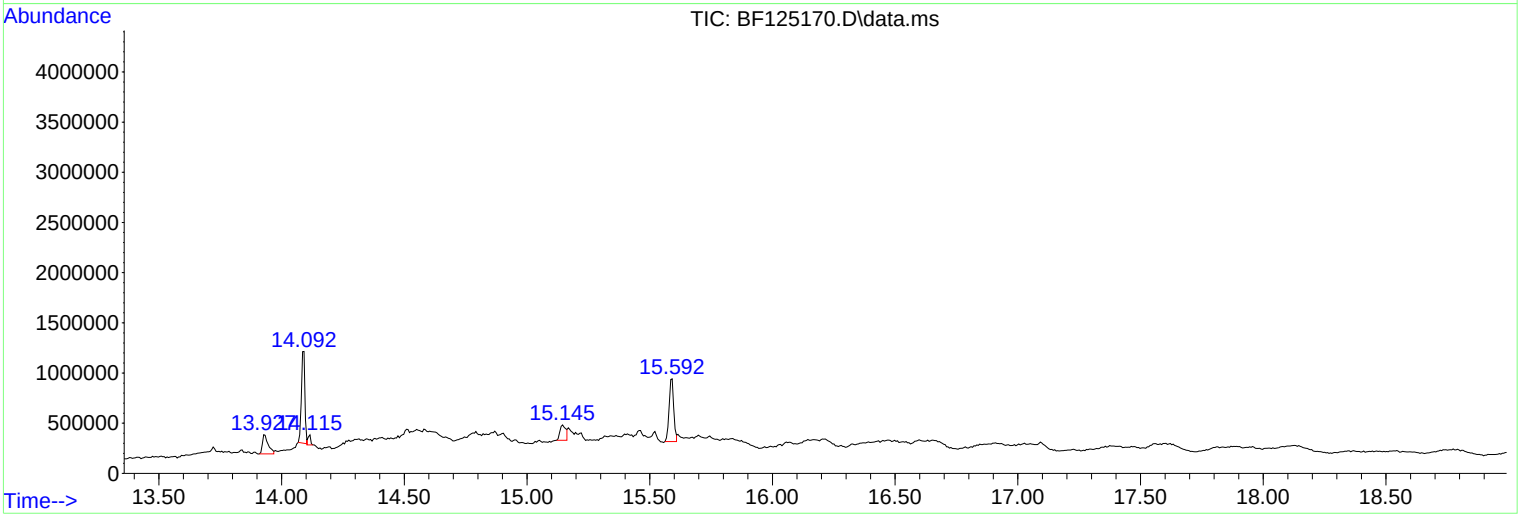
Instrument :
BNA_F
ClientSampleId :
TP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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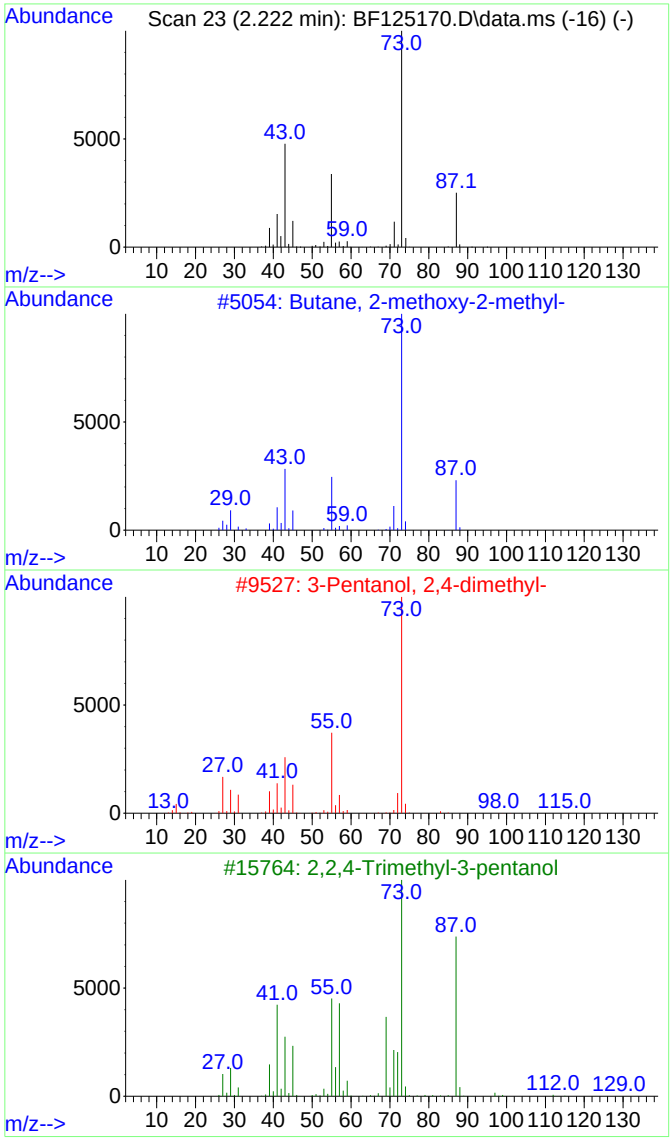
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

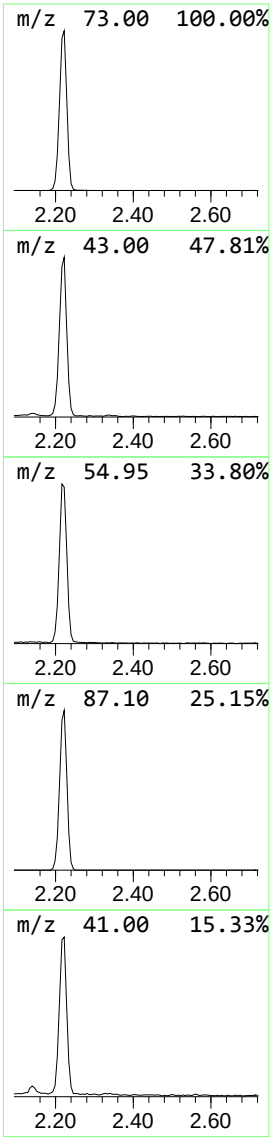
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	33.82 ng	1534490	1,4-Dichlorobenzene-d4	6.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23





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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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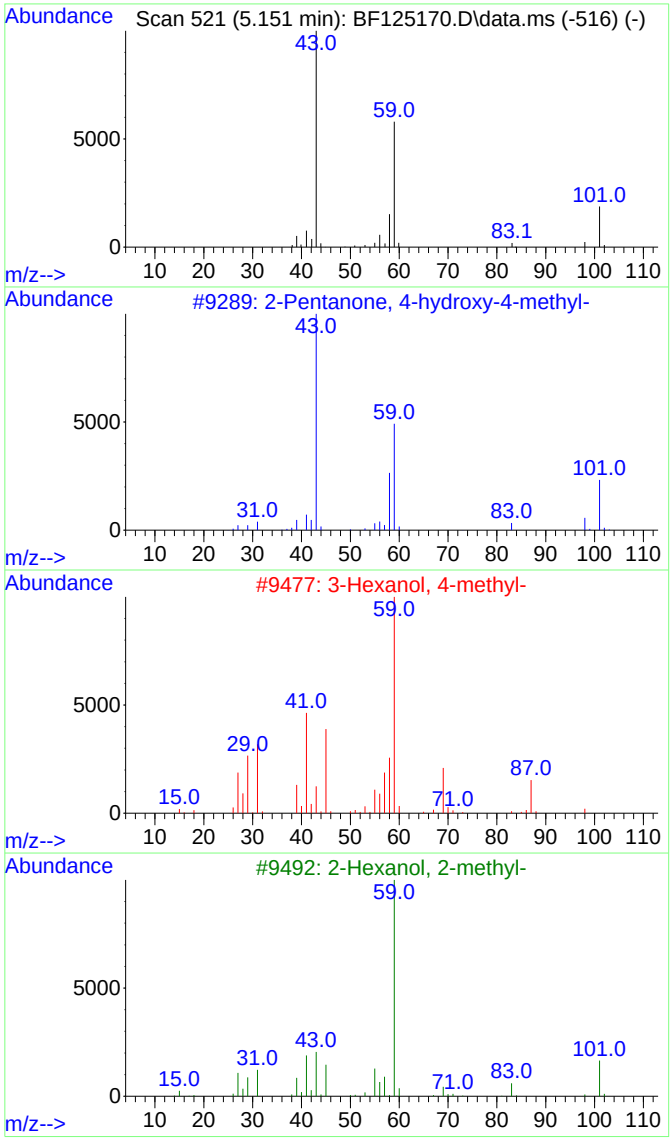
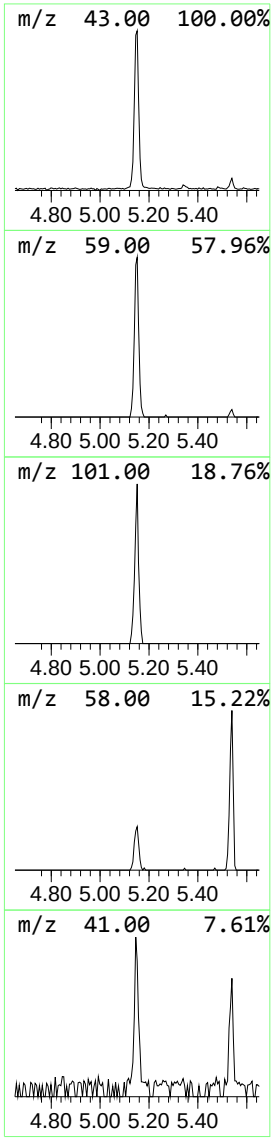
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.151	3.08 ng	139547	1,4-Dichlorobenzene-d4	6.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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Operator : JU/CG
Sample : M3449-01
Misc :
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Instrument : BNA_F
ClientSampleId : TP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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TIC Library : C:\Database\NIST20.L
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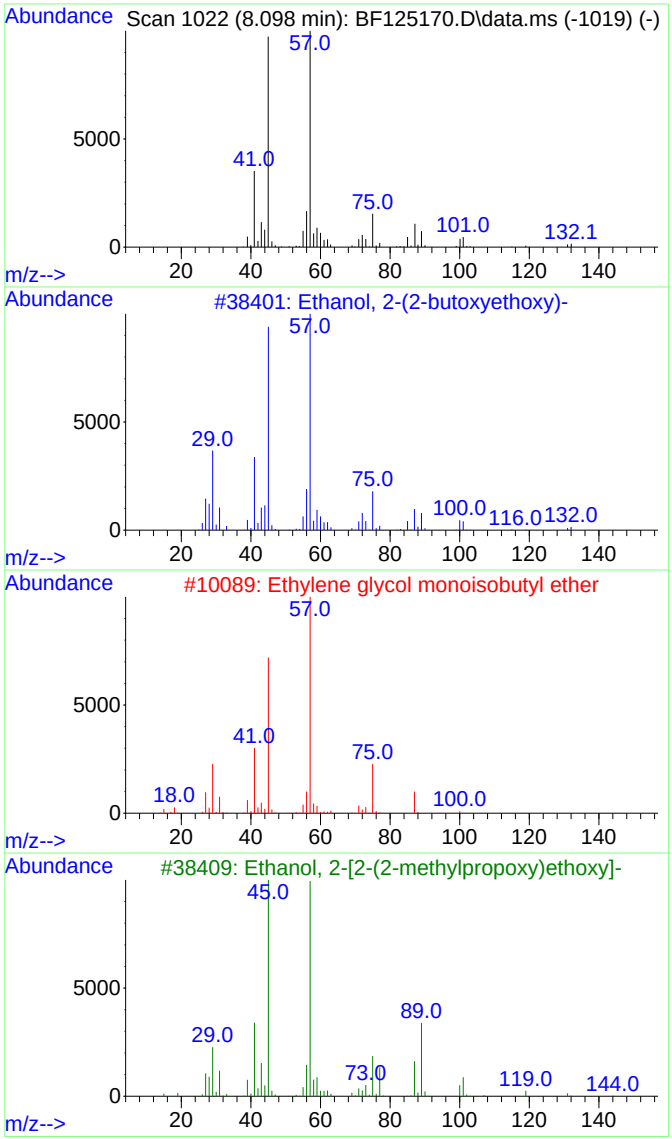
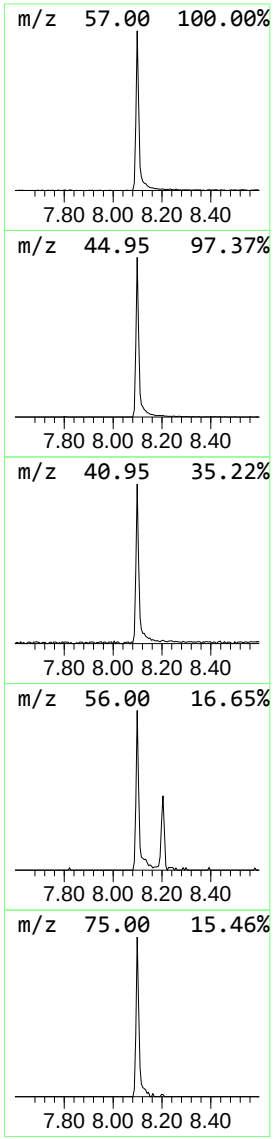
****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	8.21 ng	477278	Naphthalene-d8	8.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5	1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	47





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Instrument : BNA_F
ClientSampleId : TP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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TIC Library : C:\Database\NIST20.L
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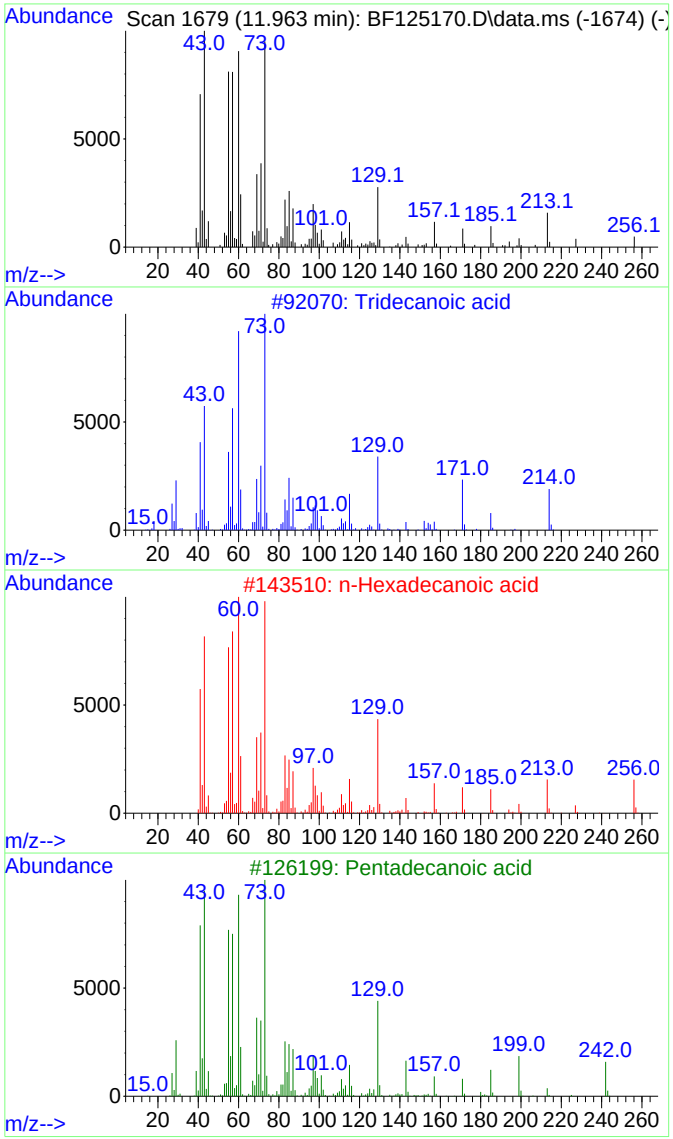
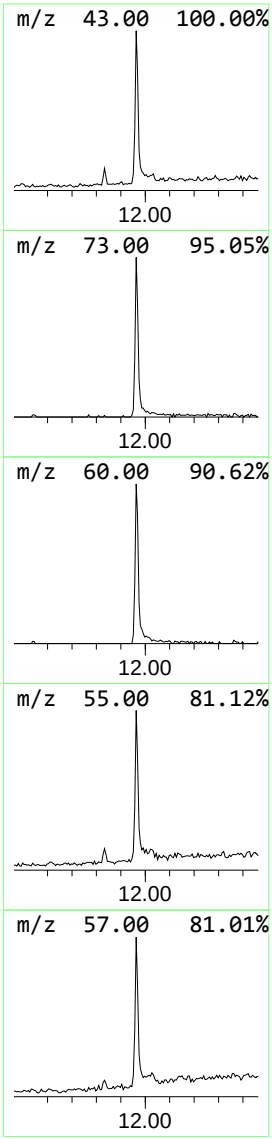
****

Peak Number 4 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.963	7.36 ng	402201	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	87
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	74





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP1

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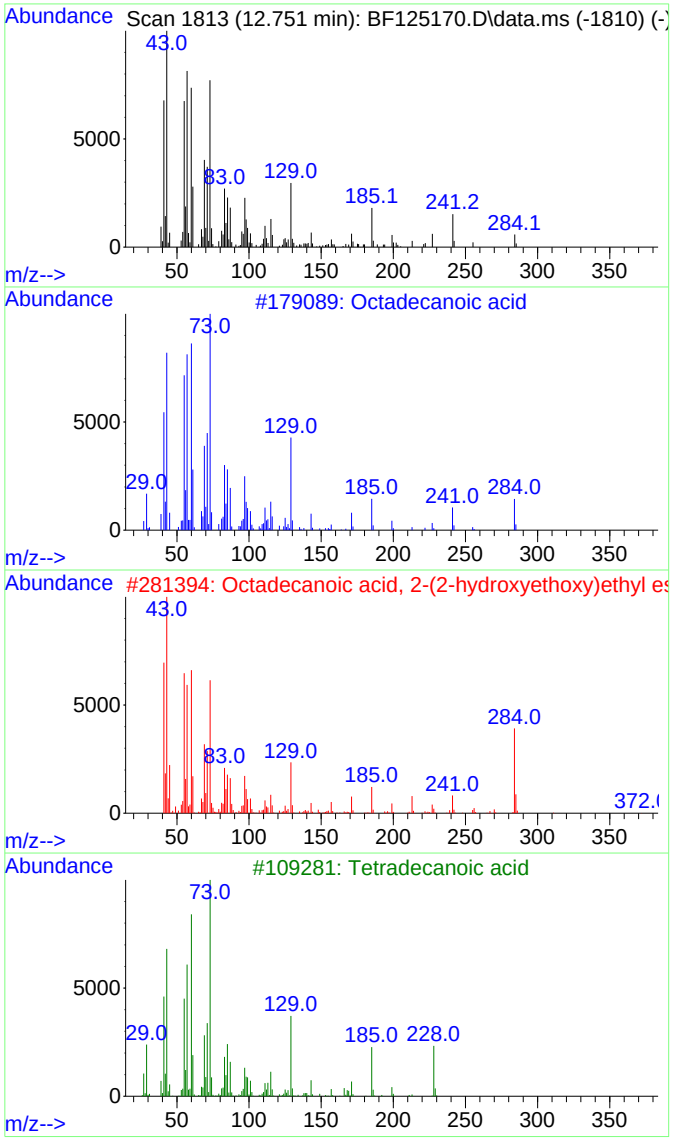
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

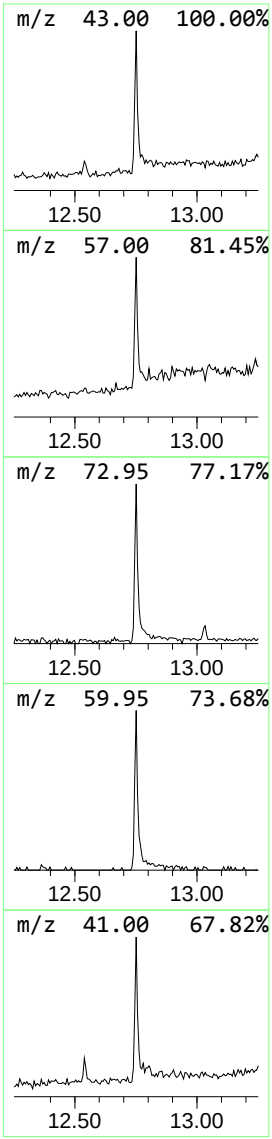
****

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.751	4.91 ng	268562	Phenanthrene-d10	11.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Undecanoic acid	186	C11H22O2	000112-37-8	60
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58





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ClientSampleId :
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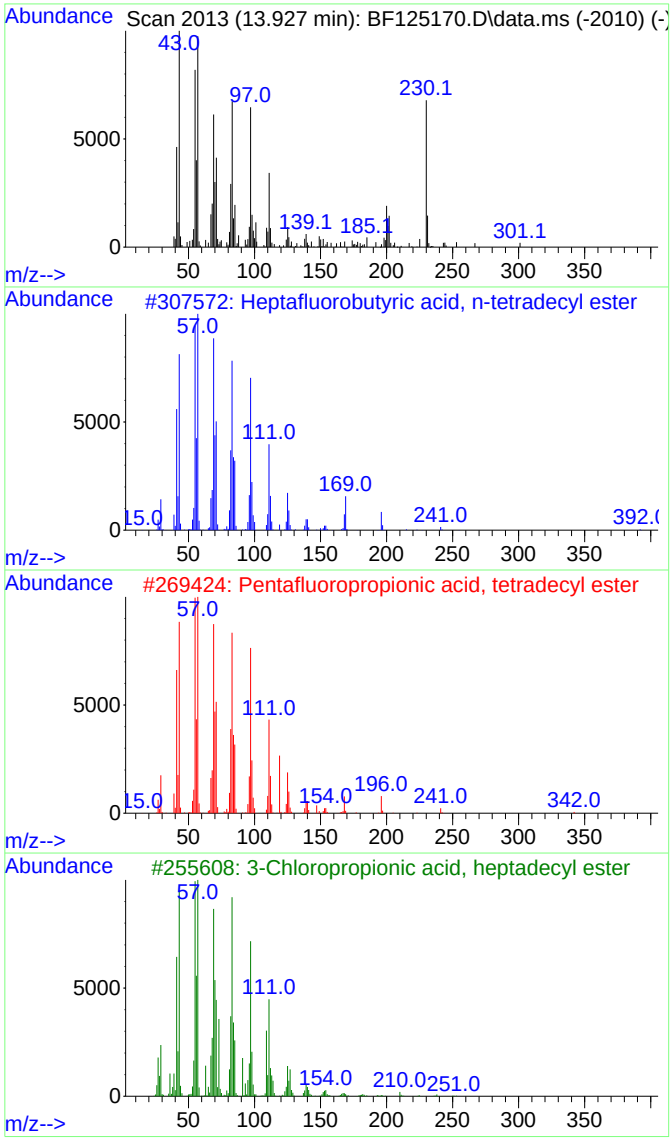
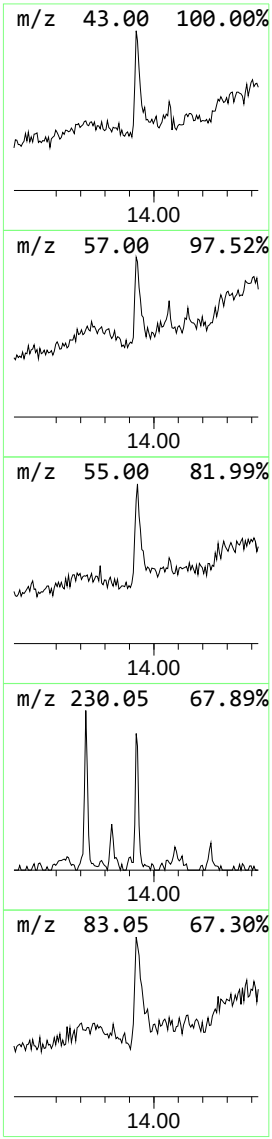
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Heptafluorobutyric acid, n-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.927	6.93 ng	313896	Chrysene-d12	14.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	70
2	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	70
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	62
4	1-Hexacosanol	382	C26H54O	000506-52-5	53
5	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	52





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.222	33.8	ng	1534490	1	6.922	907534	20.0
2-Pentanone, 4-...	5.151	3.1	ng	139547	1	6.922	907534	20.0
Ethanol, 2-(2-b...	8.098	8.2	ng	477278	2	8.204	1162350	20.0
Tridecanoic acid	11.963	7.4	ng	402201	4	11.445	1093610	20.0
Octadecanoic acid	12.751	4.9	ng	268562	4	11.445	1093610	20.0
Heptafluorobuty...	13.927	6.9	ng	313896	5	14.092	905586	20.0